Isobutyrylglycine, monoTMS

Inchi: InChI=1S/C9H21NO2Si/c1-6-8(2)10-7-9(11)12-13(3,4)5/h8,10H,6-7H2,1-5H3
InchiKey: SVKKLSFEJGDXET-UHFFFAOYSA-N
Formula: C9H21NO2Si
SMILES: CCC(C)NCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 203.35

Physical Properties

Property code	Value	Unit	Source
log10ws	0.20		Crippen Method
logp	1.753		Crippen Method
rinpol	1392.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1392.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R273348&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices